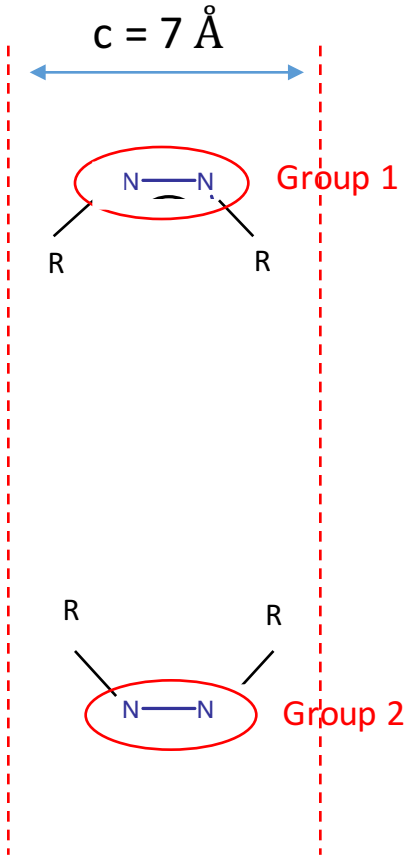
Important limitations for 1-D MOF building

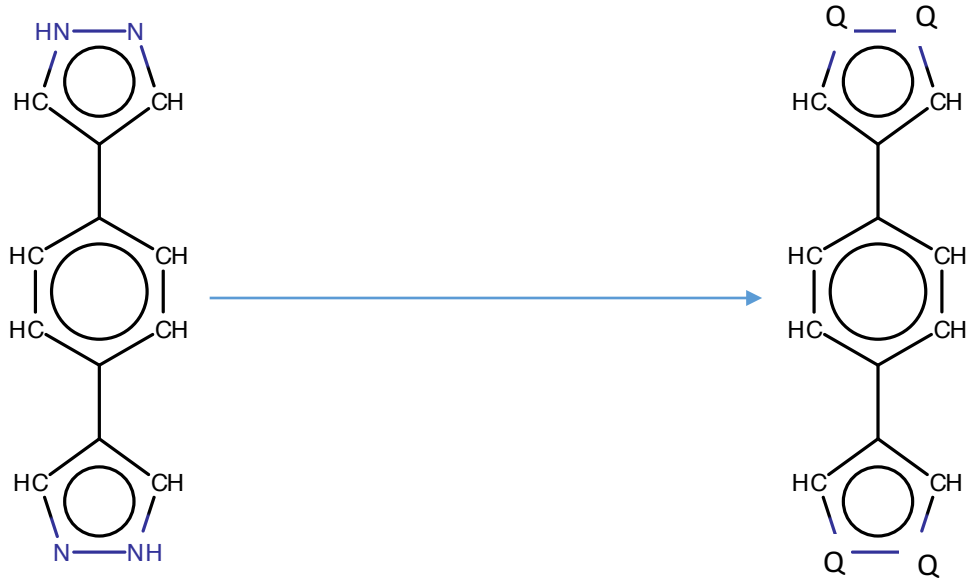
- This code strictly builds analogs of already known 1-D rod MOFs
- Therefore in the case of Fe(BDP), your ligand must adhere to the following:
  - It must have 2 connection groups, each consisting of two nitrogen atoms
  - Both N-N bonds should be parallel
  - The whole molecule should fit inside a 7 angstrom space since this is a 1-D rod MOF (basically all R groups must be oriented in such a way that they don't extend too far outside the red lines, otherwise you could have overlap with the adjacent linker in the c direction)



How to run onedMOF for Fe(bdp) analogs

5 sample assemblies are in the onedMOF/examples/ directory

- NOTE, need to pip install pycifrw which only works for me on Python2.7 for now
- Make sure FeBDP.cif and onedMOF.input are in your current working directory (Don't need to change these files)
- The *your_analog_name*.sub file in your current working directory is the molecule in xyz format to build the MOF from, with the connection atoms (N in this case) replaced by atom label Q
  - E.g.



bdp.sub

```
24
# a molecule to add to a 1-D rod MOF
C       6.924837    1.608514    4.525508
C       2.262969    7.345486    2.370767
C       7.899919    2.605668    2.823390
C       1.287866    6.348332    4.072885
C       6.801693    2.620585    3.625413
C       2.386113    6.333415    3.270862
C       5.655780    3.584125    3.533403
C       3.532026    5.369875    3.362872
C       3.942876    4.894955    4.602939
C       5.244930    4.059045    2.293335
C       5.004753    4.002080    4.688205
C       4.183053    4.951920    2.208070
H       6.300222    1.387655    5.206363
H       2.887584    7.566345    1.689911
H       8.076015    3.203670    2.106522
H       1.111791    5.750330    4.789752
H       3.497921    5.180605    5.392197
H       5.689884    3.773395    1.504077
H       5.285556    3.677497    5.535736
H       3.902250    5.276503    1.360538
Q       8.099179    0.968106    4.279773
Q       1.088627    7.985894    2.616502
Q       8.701807    1.584374    3.227808
Q       0.485999    7.369626    3.668466
```

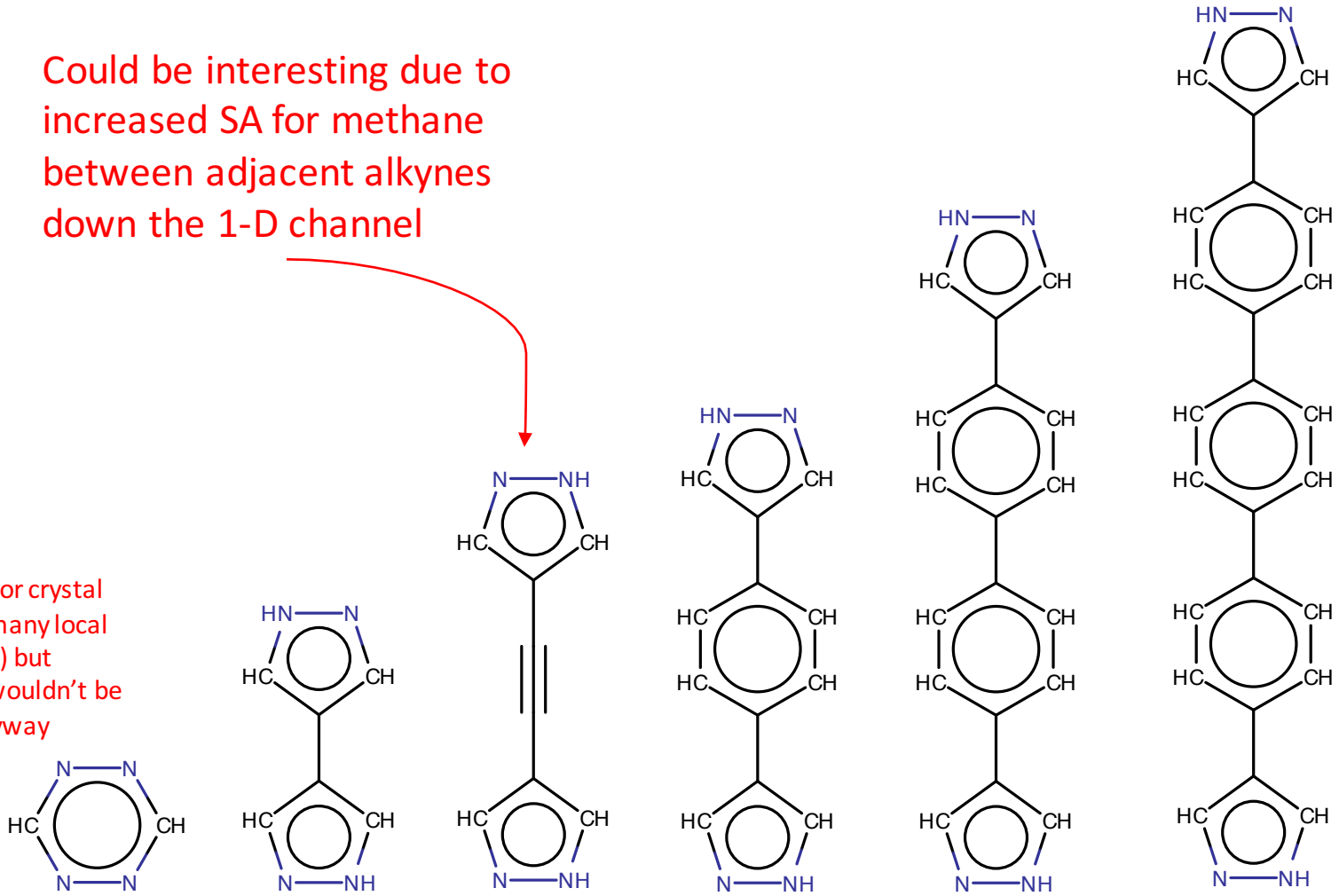
- Execute from current working directory:

python /Path/To/onedMOF/onedMOF_main.py onedMOF.input

1D MOF generator: some starting Fe(bdp) analogs

Could be interesting due to increased SA for methane between adjacent alkynes down the 1-D channel

Too small for crystal gen. (too many local minimums) but structure wouldn't be porous anyway



bdp_analog_0x1

bdp

bdp_analog_3

bdp_analog_0x0

bdp_analog_0x2

bdp_analog_2

bdp_analog_0x2: a hypothetical **1-D MOF** with a **3-D pore network**

- Can you (theoretically) set the new record for methane storage?
- Does CO2 (and not H2O?) Have a nice binding pocket in between the triple bonds?
- Does it still exhibit pressure/adsorbate induced structural phase transition?